Understanding HTS cuprates based on the phase string theory of doped antiferromagnet

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We present a self-consistent RVB theory which unifies the metallic (superconducting) phase with the half-filling antiferromagnetic (AF) phase. Two crucial factors in this theory include the RVB condensation which controls short-range AF spin correlations and the phase string effect introduced by hole hopping as a key doping effect. We discuss both the uniform and non-uniform mean-field solutions and show the unique features of the characteristic spin energy scale, superconducting transition temperature, and the phase diagram, which are all consistent with the experimental measurements of high-T_c cuprates.

The low-energy physics of high-T_c cuprates is essentially described by a doped Mott insulator [1]. The half-filling insulating phase can be well understood based on the Heisenberg model, where the bosonic resonating-valence-bond (RVB) state [2] gives a highly accurate description of both short-range and long-range spin correlations. And the mean-field bosonic RVB theory [3] provides a very useful analytic framework over a wide range of temperature.

The real challenge comes from the doped case: How the doped holes will influence the AF spin background and by doing so shape their own dynamics. A simple generalization of the aforementioned AF mean-field theory [3] to finite doping has indicated that the motion of doped holes generally gets totally frustrated at the mean-field level such that an additional spiral spin twist must be induced in order to gain a finite kinetic energy. But this is only an *artifact* due to a mistreatment of the singular phase string effect introduced by doped holes to be discussed below. We will show that the bosonic RVB ordering, which characterizes the short-range spin-spin correlations at half-filling, actually *favors* the hopping of doped holes and the RVB order parameter will still control the doped phase just like in the undoped case, a picture consistent with the original motivation for introducing the RVB concept by Anderson [1].

PHASE STRING EFFECT. The $t - J$ model in the Schwinger-boson, slave-fermion rep-resentation has the form $H_{t-J} = H_t + H_J$:

$$H_t = -t \sum_{\langle ij \rangle} \hat{H}_{ij} \hat{B}_{ji} + H.c., \qquad (1)$$

$$H_J = -\frac{J}{2} \sum_{\langle ij \rangle} \left(\hat{\Delta}_{ij}^s \right)^\dagger \hat{\Delta}_{ij}^s, \qquad (2)$$

where $\hat{H}_{ij} = f_i^\dagger f_j$, $\hat{B}_{ji} = \sum_\sigma \sigma b_{j\sigma}^\dagger b_{i\sigma}$, and $\hat{\Delta}_{ij}^s = \sum_\sigma b_{i\sigma} b_{j-\sigma}$. Here f_i is a fermionic "holon" operator and $b_{i\sigma}$ is known as the Schwinger-boson operator. At half-filling, only H_J exists and the mean-field state [3] is described by the bosonic RVB order parameter $\Delta^s = \langle \hat{\Delta}_{ij}^s \rangle$. Note that here in the slave-fermion decomposition, $c_{i\sigma} = f_i^\dagger b_{i\sigma}(-\sigma)^i$, the Marshall sign is explicitly built in through $(-\sigma)^i$ such that there is no sign σ appearing in $\hat{\Delta}_{ij}^s$. But $\hat{B}_{ji}$ in the hopping term acquires a sign σ, which would lead to $\langle \hat{B}_{ji} \rangle = 0$ in the RVB state, namely, the absence of the bare hopping for doped holes at the mean-field level.

However, if one follows the hopping of a hole continuously without making the mean-field average at first, then one finds [4] that a sequence of signs $(-1) \times (+1) \times (+1)... = (-1)^{N_c^\downarrow}$ will be picked up by the hole along its path c, where $N_c^\downarrow$ counts the total number of $\downarrow$ spins being *exchanged* with the given hole, originated from the simple sign σ mentioned above. To illustrate the importance of such a phase string effect, let us take the one hole case as an example by express-

ing the total energy as follows

$$E_{\mathbf{k}} = E_0^J - \frac{t}{N} \sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} M_{ij}, \qquad (3)$$

$$M_{ij} \equiv \sum_{\{c\},N_c^\downarrow} P[\{c\}; N_c^\downarrow](-1)^{N_c^\downarrow},$$

with using the Brillouin-Wigner formula, where E_0^J denotes the ground-state energy with the hole being *fixed* at a given lattice site. The energy gain due to the hopping comes from the second term of (3). In M_{ij} the summation runs over all the possible paths $\{c\}$ of the hole connecting i and j. The significant fact is that the weight functional P can be shown to be *positive-definite* at $E_{\mathbf{k}} < E_0^J$. (The derivation is very similar to that of the single-electron propagator in the one-hole case [4] and the details will be presented elsewhere.) It implies that the phase string factor $(-1)^{N_c^\downarrow}$ is the *only* source of phase frustration which cannot be "repaired" since $P \geq 0$, and thus is expected to dominate the low-energy physics. The only additional phase effect when there are many holes will come from the exchange of any two holes due to the fermionic nature of holons in the slave-fermion representation. At small doping, the phase string effect obviously remains dominant.

Thus the conventional slave-fermion scheme as a very successful framework at half-filling is no longer useful at finite doping if one does not know how to deal with the singular, nonlocal phase string effect [which basically counts how many ↓ (or ↑ by symmetry) spins exchanged with the hole during its propagation] hidden in the formalism. On the other hand, since the phase string effect induced by doped holes is always present in the ground state and can be "counted" in terms of the number of exchange between holons and spinons, it is possible to incorporate the singular effect explicitly into the wavefunction like the fermion statistics. It turns out that one can realize this through a unitary transformation [4] through which the $t - J$ Hamiltonian is "regulated" as the local singular sign σ is "gauged away". The resulting exact formalism is known as the phase string representation, where the RVB order parameter becomes

$$\hat{\Delta}_{ij}^s = \sum_{\sigma} \left(e^{-i\sigma A_{ij}^h} \right) \bar{b}_{i\sigma} \bar{b}_{j-\sigma}, \qquad (4)$$

while in the hopping term (1), $\hat{B}_{ji} \rightarrow \hat{B}_{ji} = \sum_{\sigma} \left(e^{i\sigma A_{ji}^h} \right) \bar{b}_{j\sigma}^\dagger \bar{b}_{i\sigma}$ and $\hat{H}_{ij} = \left(e^{iA_{ij}^f} \right) h_i^\dagger h_j$. Note that the fermionic operator f_i now is replaced by a *bosonic* holon operator h_i after the transformation while $b_{i\sigma} \rightarrow \bar{b}_{i\sigma}$ which is still a boson operator. In this new "bosonization" formalism, even though the singular sign σ in the original $\hat{B}_{ji}$ is "gauged away", the topological effect of the phase string (the total phase for a closed path) is precisely tracked by lattice gauge fields A_{ij}^f and A_{ij}^h. Here $A_{ij}^f \equiv A_{ij}^s - \phi_{ij}^0$ with $\sum_C A_{ij}^s = 1/2 \sum_{l \in C} \left(\sum_{\sigma} \sigma n_{l\sigma}^b \right)$ for a closed path C and $\sum_\square \phi_{ij}^0 = \pi$ per plaquette. And $\sum_C A_{ij}^h = 1/2 \sum_{l \in C} n_l^h$. ($n_{l\sigma}^b$ and n_l^h are spinon and holon number operators, respectively.) Here A_{ij}^s and A_{ij}^h describe quantized flux tubes bound to spinons and holons, respectively. And ϕ_{ij}^0 describes a uniform flux with a strength π per plaquette.

MEAN FIELD THEORY. In the phase string formulation, the hopping term becomes finite as $\langle \hat{B}_{ji} \rangle \neq 0$ [5] when $\Delta^s \neq 0$. Namely, the single RVB field Δ^s will still be the only order parameter that controls both the undoped and doped phases. Note that Δ^s decides the short-range spin-spin correlations as shown in the relation $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = -1/2|\Delta^s|^2$ for nearest-neighboring i and j.

In the following let us focus on the so-called uniform-phase solution where holons and spinons are assumed to distribute homogeneously without the phase separation. In the ground state, the bosonic holons will experience the Bose condensation (BC) such that one may replace A_{ij}^h by $\bar{A}_{ij}^h$ satisfying $\sum_\square \bar{A}_{ij}^h = \delta\pi$ (δ is the doping concentration) and $A_{ij}^f \rightarrow -\phi_{ij}^0$ as A_{ij}^s diminishes due to the pairing of spinons with a gap opening (see below). Then the mean-field state can be straightforwardly obtained.

Fig. 1 illustrates how the spin dynamics evolves into the metallic regime: the spin dynamic susceptibility at (π,π), $\chi_{\pi\pi}''(\omega)$, is shown at $\delta = 0$

and $\delta = 1/7 \approx 0.143$, respectively. Compared to half-filling, a resonance-like single peak emerges at a finite energy E_g with the weight diminishes below it. The inset shows the doping-dependence of E_g which peaks at $\sim 0.4J$ (independent of t) around $\delta \sim 0.2$, which is very close to the famous $41meV$ peak observed [6] in optimal $YBCO$ compound by neutron scattering (for $J \sim 100meV$). E_g decreases monotonically with reducing δ in low-doping regime.

The phase string effect is solely responsible for such a resonance-like peak through the gauge field $\bar{A}_{ij}^h$. Another unique prediction of the phase string effect is shown in Fig. 2 for the local susceptibility $\chi_L''(\omega) = 1/N \sum_{\mathbf{q}} \chi''(\mathbf{q},\omega)$ which shows multi-peak structure at higher energies like Landau levels as $\bar{A}_{ij}^h$ describes uniform fictitious flux seen by spinons. Note that the high-energy peaks are contributed by those spin fluctuations away from the AF momentum (π,π) in momentum space and are only significant under the integration over the whole Brillouin zone, which remains to be seen experimentally in the uniform phase like the optimal-$YBCO$ compound.

Another interesting property is that the ground state is intrinsically a superconducting state with d-wave symmetry. This can be verified by the
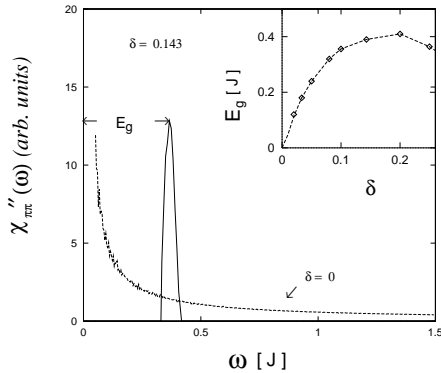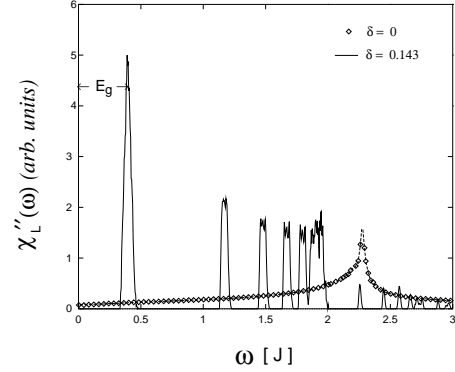

Figure 2. Local dynamic spin susceptibility as the function of energy

paring order parameter [5]

$$\Delta_{ij}^{SC} = \Delta^s f_{ij} h_0^2 \left\langle e^{-\frac{i}{2}(\Phi_i^s + \Phi_j^s)} \right\rangle \qquad (5)$$

for nearest-neighboring sites i and j. Here the numerical factor f_{ij} changes sign from $j = i \pm \hat{x}$ to $j = i \pm \hat{y}$ determining the d-wave symmetry, $h_0 = \langle h_i^\dagger \rangle$, and the phase Φ_i^s is defined as

$$\Phi_i^s = \sum_{l \neq i} \text{Im} \ln (z_i - z_l) \sum_\alpha \alpha n_{l\alpha}^b \qquad (6)$$

which describes vortices (anti-vortices) centered at up (down) spinons. The vortices-antivortices described by Φ_i^s are all paired up in the ground state to ensure a finite Δ_{ij}^{SC}. But at finite temperature, free vortices appear in Φ_i^s as spinons are thermally excited will eventually kill the superconducting condensation. Using the effective Hamiltonian for holon $H_h = -t_h \sum_{\langle ij \rangle} \hat{H}_{ij} + h.c.$, T_c can be estimated [5] as the temperature at which the excited spinon number equals to the total holon number. Fig. 3 show the correlation between T_c and the spin characteristic energy E_g which is consistent with the experimental relation for the cuprate superconductors [7,8]. In particular, $T_c \sim 100K$ at $\delta = 0.143$ with $E_g \sim 40meV$ without tuning parameters except for $J \sim 100meV$.

The phase diagram of the present mean-field theory is illustrated in Fig. 4. Note that the

Figure 1. Dynamic spin susceptibility at the AF vector (π,π) as the function of energy.

whole theory is underpinned by the RVB order parameter Δ^s controlling the nearest-neighboring AF spin correlations which are gradually reduced with the increase of δ. Both AF long-range ordering in the insulating phase (holes must be localized) and superconducting condensation in metallic phase occur inside such an RVB background, characterized by the BCs of spinons and holons, respectively. Note that there is an underdoped metallic regime denoted by SBC in Fig. 4 under the dashed curve which indicates the case of spinon BC in the metallic phase, corresponding to a non-uniform solution of the present mean-field theory [5]. In the above uniform phase, the spin gap E_g shown in Fig. 1 prevents the BC of spinons. But a non-uniform distribution of holons will lead to a spatial redistribution of the fictitious flux seen by spinons through A_{ij}^h to generate a low-energy tail in spinon spectrum. At low doping, the Bose condensation of spinons can happen as the tail extends to zero, which physically means short-range AF orders exist in the hole-dilute regions. Whether such a solution is a micro or macro phase separation still needs further investigation. But generally the dynamic spin susceptibility function will show a double-peak structure in energy space near (π, π) with a pesudo-gap feature as there always will be some
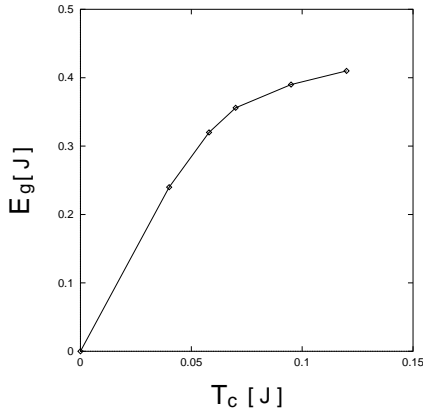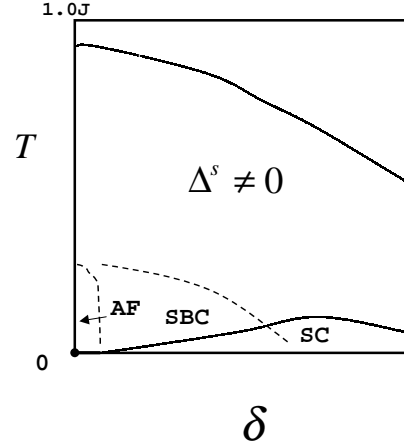

Figure 4. Phase diagram of the RVB state characterized by Δ^s: AF and SC phases correspond to spinon and holon Bose condensations, respectively. And SBC denotes the spinon Bose condensation in the metallic regime.

weight extends towards the zero energy limit [5]. This fact may have already seen experimentally in the underdoped $YBCO$ compounds [7,8].

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Figure 3. Relation between the spin energy E_g (Fig.1) and T_c.